# Sharing polarization within quantum subspaces

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Given an ensemble of $n$ spins, at least some of which are partially polarized, we investigate the sharing of this polarization within a subspace of $k$ spins. We assume that the sharing results in a pseudopure state, characterized by a single purity parameter which we call the bias. As a concrete example we consider ensembles of spin-1/2 nuclei in liquid-state nuclear magnetic resonance (NMR) systems. The shared bias levels are compared with some current entanglement bounds to determine whether the reduced subspaces can give rise to entangled states.

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## I. INTRODUCTION

Liquid-state nuclear magnetic resonance (NMR) techniques have proved a convenient test-bed for implementing quantum algorithms [1, 2, 3, 4, 5, 6]. However, a conventional NMR quantum computer starts off in an initial state which is very similar to a maximally mixed state, due to the tiny population differences between the energy levels of the spin-1/2 nuclei which act as the qubits [7, 8].

Various approaches to this initialization problem have been suggested. Firstly, it is possible to convert thermal states into pseudopure states [1, 2]: this approach has been adopted in the vast majority of NMR implementations of QIP, but is not scalable [8]. Secondly, non-Boltzmann distributions can be prepared, for example with *para*-hydrogen [9, 10, 11], giving almost pure states which lie above the entanglement threshold [12]. Thirdly, computational schemes have been described [13, 14, 15] which concentrate the small polarization available on a large number of spins into a smaller subspace.

Here we investigate the effects of polarization sharing on achieving states of useful purity. The schemes mentioned above *concentrate* polarization onto a *smaller* subset of spins, but we study the effects of spreading the polarization over a *larger* subset of spins. We assume that the polarization sharing results in a pseudopure state with a purity characterized by a bias parameter $\delta$ that we define below. The bias is then compared with known entanglement bounds derived for pseudopure states.

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## II. PSEUDOPURE STATES AND ENTANGLEMENT

In the high temperature approximation, the initial state of a (homonuclear) NMR quantum computer is

$$\rho_{eq} \approx \frac{1}{2^n}\left(\mathbf{1}_n + \frac{B}{2}\sum_{j=1}^{n}\sigma_{iz}\right), \tag{1}$$

where $n$ is the total number of spins, $\mathbf{1}_n$ is the identity matrix of order $2^n$, $B = -\hbar\omega/k_BT$ is a Boltzmann factor and $\sigma_{jz}$ is the $z$ Pauli matrix for spin $j$. A standard implementation of an algorithm requires the quantum computer to start off in a pure state, characterised by having a single non-zero eigenvalue, of size one. Clearly, the thermal state (1) has many different eigenvalues and so to prepare pure from thermal states, a non-unitary process must be employed at some stage. Cooling to the ground state is an example of such a process, but is ineffective in NMR due to the small energy gaps involved. Pseudopure $k$-qubit states have an eigenvalue spectrum between these extremes, having one large eigenvalue and $2^k - 1$ degenerate smaller eigenvalues. This means that thermal states can be converted into pseudopure states by particularly simple non-unitary processes, such as averaging $2^k - 1$ population terms.

A general $k$-qubit pseudopure state $\chi$ takes the form

$$\chi_{k,\delta} = (1-\delta)\frac{\mathbf{1}_k}{2^k} + \delta|\psi\rangle\langle\psi|, \tag{2}$$

with dynamics identical to those of the corresponding pure state $|\psi\rangle\langle\psi|$. (We explicitly use the symbol $\chi$ to denote pseudopure states.) The state is characterised by a single parameter, $\delta$, which we call the bias of the state.

Another useful description is to write out the pseudopure state explicitly in its eigenbasis with the eigenvalues in descending order to give

$$\chi_{k,\delta} = \mathrm{Dg}[f, \overbrace{\frac{1-f}{2^k-1}, \frac{1-f}{2^k-1}, \ldots, \frac{1-f}{2^k-1}}^{(2^k-1)\ \text{terms}}] \tag{3}$$

where Dg[...] denotes a diagonal matrix and $f$ is both the fractional population of the desired state $|\psi\rangle\langle\psi|$ and the *largest* eigenvalue and is related to the bias by

$$\delta = \frac{2^k f - 1}{2^k - 1}. \tag{4}$$

A pseudopure state will always be separable if $\delta$ is less than some critical value, and Braunstein *et al.* [16] have described upper and lower bounds on separability. A state of the form given in Eq. 2 was shown to be explicitly separable for sufficiently small biases such that

$$\delta \leq \delta_l = \frac{1}{1 + 2^{2k-1}} \tag{5}$$

and we say that these states belong to the region **S**. If the bias exceeds their upper bound

$$\delta > \delta_u = \frac{1}{1 + 2^{\frac{k}{2}}} \tag{6}$$

the state is said to lie in the entangled region **E**, or more appropriately the *entanglable* [17] region. In the region in between, **ES**, it is not known whether entangled states can be prepared. These bounds were subsequently improved, shrinking the size of **ES**. For example, Gurvits and Barnum [18] have tightened the lower bound to

$$\delta_l = \frac{3}{2(6)^{k/2}}. \tag{7}$$

Current NMR implementations with Boltzmann initialization use states lying in the separable region **S** and it seems possible to enter the region **ES** only by employing more qubits. For example, using the Gurvits–Barnum lower bound with a typical Boltzmann factor of $B = 10^{-5}$, the state will cross over into **ES** for $k \geq 41$.

Similar themes have been taken up by other authors as well. Yu *et al.* have shown [17] that by using unitarily transformed thermal states in place of pseudopure states, the **ES** to **E** transition can take place with a smaller number of qubits: making pseudopure states from thermal states involves convex mixing and, therefore, decreases the likelihood of entanglement. Other researchers have shown [19] that entanglement can also exist in a $2 \times N$ dimensional quantum system, when *only* the qubit is pure and the $N$ dimensional system is in a highly mixed state, such as a two level atom interacting with a high temperature field.

Here we investigate the *sharing* of polarization within a pseudopure quantum subspace. We consider an initial state

$$\rho_{n,p,\sigma} = \left(\bigotimes_{j=1}^{p} \phi_\sigma\right) \otimes \left(\bigotimes_{j=p+1}^{n} \mathbf{1}_1/2\right) \tag{8}$$

where $n$ is the total number of qubits of which $p$ qubits are in the state,

$$\phi_\sigma = \begin{pmatrix} (1+\sigma)/2 & 0 \\ 0 & (1-\sigma)/2 \end{pmatrix}, \quad 0 \leq \sigma \leq 1, \tag{9}$$

having a polarization $\sigma$ and the remaining $n-p$ qubits are maximally mixed. Our goal is to compute the achievable bias in a $k$ qubit pseudopure state where $k \leq n$, *i.e.*, we are interested in the transformation $\rho_{n,p,\sigma} \mapsto \chi_{k,\delta}$. We achieve this in two steps: (a) convert $\rho_{n,p,\sigma}$ into a $k$ qubit state $\tau_k$ using a partial trace operation, and then (b) convert $\tau_k$ into a pseudopure state $\chi_{k,\delta}$ using cyclic averaging.

For simplicity consider a state $\rho_{n,p,1}$ with all the $p$ qubits being perfectly polarized,

$$\begin{aligned} \rho_{n,p,1} &= \left(\bigotimes_{j=1}^{p} |0\rangle\langle 0|\right) \otimes \left(\bigotimes_{j=p+1}^{n} \mathbf{1}_1/2\right) \\ &= \frac{1}{2^{n-p}} \mathrm{Dg}[\overbrace{1, 1, \ldots, 1}^{2^{n-p}\ \text{terms}}, 0, 0, \ldots, 0]. \end{aligned} \tag{10}$$

and consider the case $k = p$. Partially tracing [20] out the $n-k$ qubits from $\rho_{n,p,1}$ leaves us with the $k$ qubit reduced state

$$\tau_k = \mathrm{Dg}[1, \overbrace{0, 0, \ldots, 0}^{2^k-1\ \text{terms}}]. \tag{11}$$

This is also a pseudopure state $\chi_{k,1}$ with maximum achievable bias of one. The partial trace operation reduces the dimensionality of the system and for a diagonal state, is equivalent to taking partial sums of consecutive eigenvalues along the ordered diagonal. Physically, it just corresponds to ignoring the $n-k$ qubits. In the case of $k = p$, the reduced subspace after the partial trace operation is already a (pseudo)pure state, with $\delta = 1$. This will also be the case when $k < p$. However, for $p < k \leq n$, the reduced state $\tau_k$ will have several different eigenvalues.

We can explicitly generate the desired pseudopure state by writing the mixed state in its ordered eigenbasis and then averaging over cyclic permutations of the $2^k - 1$ trailing elements. This procedure (which can be considered as a generalisation of the twirl operation [21]) is experimentally implementable by exhaustive temporal averaging [22]; more efficient procedures are also available [22, 23]. A non-unitary process cannot increase the maximum eigenvalue of a state $\tau$, but by definition, a pseudopure state has only one non-degenerate eigenvalue which must coincide with the maximum eigenvalue of $\tau$. Cyclic averaging leaves this eigenvalue unchanged and therefore extracts the maximum bias $\delta$.

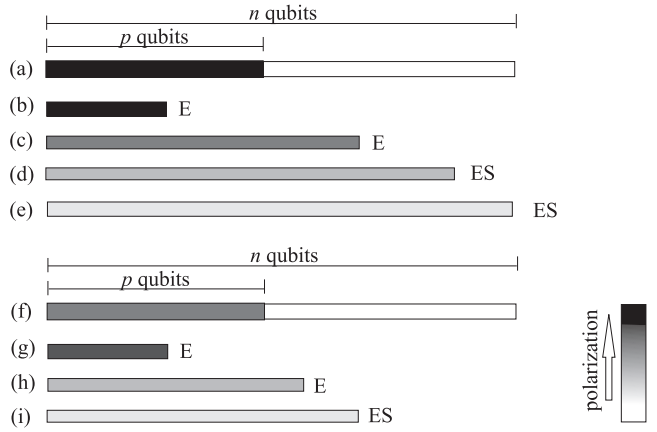


FIG. 1: The effect of sharing the polarization of $p$ pure [(a)–(e)] or partially pure [(f)–(i)] spins on quantum subspaces. Starting with $p$ pure spins (a), we can *pick* $k \leq p$ pure spins (b) and extract all the available polarization. The polarization can also be *spread* onto a bigger subspace while retaining the entanglability (c). Sharing the polarization within even higher dimensional subspaces decreases the resulting bias and therefore the possibility of entanglement, (d) and (e). As the size of the extracted subspace increases, the bias drops exponentially. Smaller biases are shown by lighter tones of grey. For $p$ partially polarized spins (f), we can *concentrate* the bias onto smaller subspaces (g) or spread it onto bigger subspaces, (h) and (i), with a corresponding decrease in the bias reducing the likelihood of entanglement.

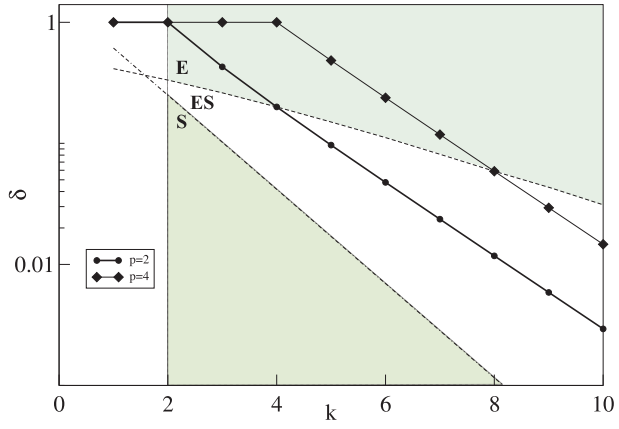


FIG. 2: (Color online) Sharing the polarization of 2 and 4 pure spins. The upper shaded region is **E** and the lower shaded region is **S**, whereas **ES** is in between. The border between two regions belongs to the less entangled region. The regions are intended to guide the eye, and are only shown for 2 or more spins, where the concept of entanglement is valid.

Algebraic manipulation shows that the maximum eigenvalue of $\chi_{k,\delta}$ is given by the formula

$$f = \frac{\mathrm{Tr}(\rho_{n,p,\sigma}\rho_{n,k,1})}{\mathrm{Tr}(\rho_{n,k,1}^2)} = \frac{1}{2^{n-k}}\mathrm{Tr}(\rho_{n,p,\sigma}\rho_{n,k,1}) \qquad (12)$$

which is the overlap between the states (8) and (10). Note that we do not consider here precisely *how* the polarization sharing procedures might be implemented in practice, but simply determine the limits. Our results are summarised in Fig. 1 and exemplified below.

## III. PERFECTLY POLARIZED QUBITS

Considering the form of Equation 10 ($n$ spins out of which $p$ are perfectly polarized and the rest are maximally mixed), we see that $f$ is given by

$$f = \begin{cases} 2^{p-k} & \text{for } k \geq p \\ 1 & \text{for } k < p \end{cases} \qquad (13)$$

and from Equation 4 the achievable bias is

$$\delta = \begin{cases} \frac{2^p-1}{2^k-1} & \text{for } k \geq p \\ 1 & \text{for } k < p. \end{cases} \qquad (14)$$

For $k < p$, *all* the purity can be extracted as this is equivalent to picking out the pure spins from a set of pure and maximally mixed spins. The case $k > p$ is more interesting as this involves distributing the polarization of $p$ spins over a larger subspace and is the polarization sharing that we shall be mainly interested in. Figure 2 shows the results for $p$ pure spins, with $p = 2$ and 4. For $k > p$, the bias falls off exponentially as $k$ is increased.

Examining Equation 10 also shows that adding extra qubits (increasing $n$) neither hinders nor helps the extraction of purity onto qubits; it seems that the only role of $n$ is that it limits the number of spins in the pseudopure subspace, as evidently $k \leq n$. Of course these additional qubits may assist the implementation of the manipulations necessary to prepare the pseudopure state, but they have no ultimate effect on the extracted bias.

The biases of the $k$-qubit pseudopure subspaces can now be compared with the entanglement bounds, but for the possibility of entanglement to arise in the first place, the pure component in the pseudopure state must be entangled. For example, the direct product 2-qubit state $|00\rangle\langle 00|$ is pure, but is clearly separable. However, one can always find a unitary operator that converts an arbitrary pure state into any desired pure target state, be it entangled or otherwise. Any pure state is therefore *unitarily equivalent* to an entangled state of the same dimensions, and we can assume that our $k$-qubit pseudopure state comprises a pure, entangled component mixed in with the maximally mixed state. This is the justification for using the term *entanglable* for the region **E**, as mentioned in the previous Section.

For $k \leq p$, the $k$-qubit subspace is obviously in the region **E** but for $k > p$, increasing $k$ leads to an exponential drop in the extractable bias $\delta$. At some critical $k$ we step into the region **ES**. This transition from **E** to **ES** takes place where $\delta = \delta_u$, which can be identified in Figure 2 as the point at which the bias curve crosses into

the region **ES**, and occurs at $k_c = 2p$. What this means is that if we start with $p$ perfectly polarized spins, then for $k < 2p$ our extracted system will be in **E**. However, for higher values of $k$ we shall be in **ES**. We also note that as a result of this polarization sharing we will never enter **S**; this is clear from the slopes of the lines in the figures, and a simple proof is given in the Appendix.

## IV. PARTIALLY POLARIZED QUBITS

We now generalize the above example to consider $p$ spins that are not perfectly polarized, each having a uniform non-zero polarization $0 < \sigma < 1$. The $n$-qubit state $\rho_{n,p,\sigma}$ is now given by

$$\begin{aligned}\rho_{n,p,\sigma} &= \left(\bigotimes_{j=1}^{p}\left\{\left\{\frac{1+\sigma}{2},\frac{1-\sigma}{2}\right\}\right\}\right)\otimes\left(\bigotimes_{j=p+1}^{n}\frac{\mathbf{1}_1}{2}\right)\\ &= \frac{1}{2^{n-p}}\left\{\left\{\overbrace{\left(\frac{1+\sigma}{2}\right)^p}^{2^{n-p}\text{ terms}},\overbrace{\left(\frac{1+\sigma}{2}\right)^{p-1}\left(\frac{1-\sigma}{2}\right)}^{(2^{n-p}\ {}^pC_1)\text{ terms}},\right.\right.\\ &\left.\left.\ldots,\overbrace{\left(\frac{1+\sigma}{2}\right)\left(\frac{1-\sigma}{2}\right)^{p-1}}^{(2^{n-p}\ {}^pC_{p-1})\text{ terms}},\overbrace{\left(\frac{1-\sigma}{2}\right)^p}^{2^{n-p}\text{ terms}}\right\}\right\},\end{aligned} \tag{15}$$

where ${}^lC_j = l!/j!(l-j)!$ is the binomial coefficient. If $k \geq p$, calculating $f$ involves summing only the first $2^{n-k}$ terms, each being of the same size $((1+\sigma)/2)^p$. This is best illustrated with a numerical example. Consider a state with $n = 4$ and $p = 2$

$$\rho_{4,2,\sigma} = \frac{1}{4}\,\mathrm{Dg}[\overbrace{\left(\frac{1+\sigma}{2}\right)^2}^{4\text{ terms}},\overbrace{\left(\frac{1-\sigma}{2}\right)\left(\frac{1+\sigma}{2}\right)}^{8\text{ terms}},\overbrace{\left(\frac{1-\sigma}{2}\right)^2}^{4\text{ terms}}] \tag{16}$$

and suppose we want to share the purity over a 3-qubit subspace ($k = 3$). Calculating $f$ will only involve a partial sum of the first $2^{n-k} = 2$ terms in (16), each of these terms being $(1/4)((1+\sigma)/2)^2$. Similarly if $k = 2$, we need a partial sum over the first 4 terms and for $k = 4$, we need to consider just the first term. In each of these cases only the leading terms are involved in the partial sums, and we can derive a formula for $f$

$$f = 2^{-k}(1+\sigma)^p \tag{17}$$

with a corresponding bias

$$\delta = \frac{(1+\sigma)^p - 1}{2^k - 1}. \tag{18}$$

If $k < p$ we are concentrating polarization onto a subspace smaller than the original, and can expect to extract a higher bias. in this case the overlap and bias must be calculated explicitly on a case by case basis. We do not consider this polarization concentration further.

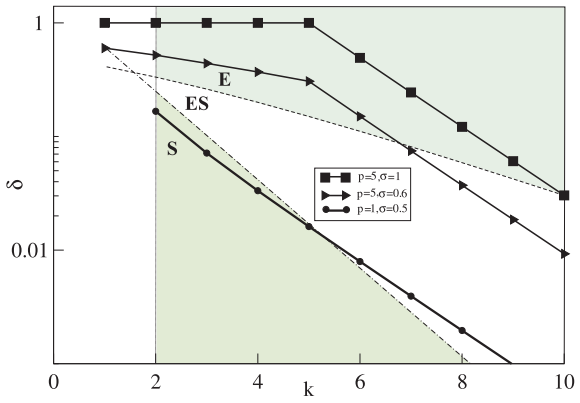


FIG. 3: (Color online) Sharing the polarization of impure spins. The regions **E**, **ES** and **S** are highlighted in the same way as in Fig. 2. The figure demonstrates polarization sharing for 5 pure and 5 impure spins. The effect of sharing from a single weakly polarized spin is also shown; when shared over 6 or more spins the state moves from being provably separable into the region where it is unknown whether or not it may be entangled.Note, however, that states currently placed in **ES** may subsequently move to **S** if lower bounds are further tightened.

As with perfectly polarized spins, sharing from impure spins also entails an exponential decrease in the extractable bias as the size of the subspace $k$ increases. The critical size $k_c$ for impure states at which the state is no longer provably entangled is now given by

$$k_c = \lceil 2p\frac{\ln(1+\sigma)}{\ln 2}\rceil \tag{19}$$

where $\lceil x\rceil$ represents the next higher integer to $x$ (only integral numbers of spins are possible). It is straightforward to see that with $p$ partially polarized spins, polarization can be shared over a smaller number of qubits than when the $p$ spins are ideally polarized, as shown in Figure 2.

## V. CONCLUSIONS

In this paper, we have shown that given $p$ perfectly polarized spins, we can share polarization among $2p-1$ spins, such that their bias keeps them in the provably entangled region. For example, for $p = 2$ pure spins, we can spread the polarization over 3 spins, while "protecting" the entanglement. Similar results can be achieved when the initial spins are not completely polarized: from (19), we find that for $\sigma \geq (\exp(3\ln 2/4) - 1) \approx 0.682$, it is possible to spread the polarization of 2 qubits onto a higher spin subspace. Our results suggest that polarization sharing is of limited value with only a single pair of protons from *para*-hydrogen added onto our substrate

molecule [9], but show more promise for a higher number of molecules $M$. Preparing such molecules is in principle possible and we are currently investigating approaches for such multi-qubit systems.


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## APPENDIX

When sharing polarization from $p$ pure qubits, the system always lies within the regions **E** and **ES**, never entering the explicitly separable region **S**. To prove this we must show that the extracted purity is always greater than the Gurvits–Barnum bound,

$$\frac{2^p-1}{2^k-1} > \frac{3}{2(6)^{k/2}}; \qquad \forall\ k \geq p. \tag{A.1}$$

*Proof.* The left hand side of Equation A.1 will be a minimum when $p = 1$, and so it suffices to prove this extreme case:

$$\frac{1}{2^k-1} > \frac{3}{2(6)^{k/2}}. \tag{A.2}$$

Now the L.H.S. of (A.2) is clearly greater than $1/2^k$. So the inequality will be true when the ratio of $1/2^k$ and right hand side of (A.2) is greater than unity. This ratio $(2/3)^{1-k/2}$ is greater than one for $k > 2$, whereas (A.2) can also be shown to be correct for $k = 2$ by explicit calculation. □


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